



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2022 – 06:20 PM JST

PDB ID : 7F22
Title : L-lactate oxidase with pyruvate
Authors : Morimoto, Y.; Inaka, K.
Deposited on : 2021-06-10
Resolution : 1.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

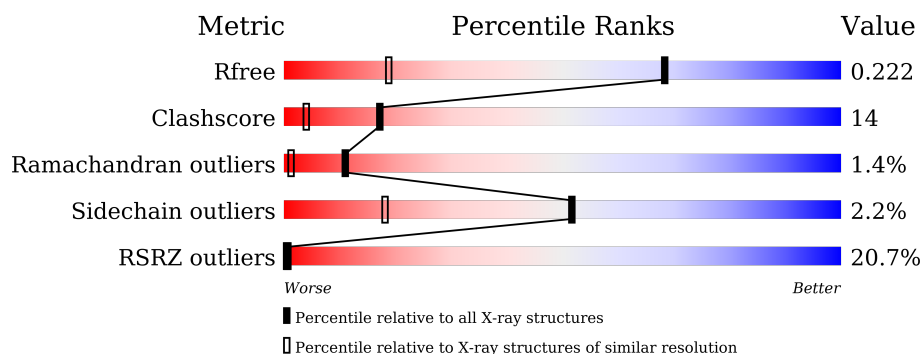
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.41 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2579 (1.44-1.40)
Clashscore	141614	2696 (1.44-1.40)
Ramachandran outliers	138981	2632 (1.44-1.40)
Sidechain outliers	138945	2631 (1.44-1.40)
RSRZ outliers	127900	2528 (1.44-1.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	736	
1	B	736	

2 Entry composition [i](#)

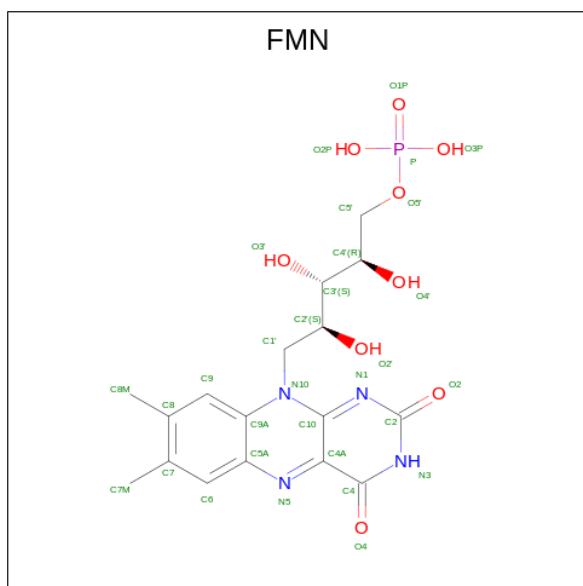
There are 4 unique types of molecules in this entry. The entry contains 6496 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called L-lactate oxidase.

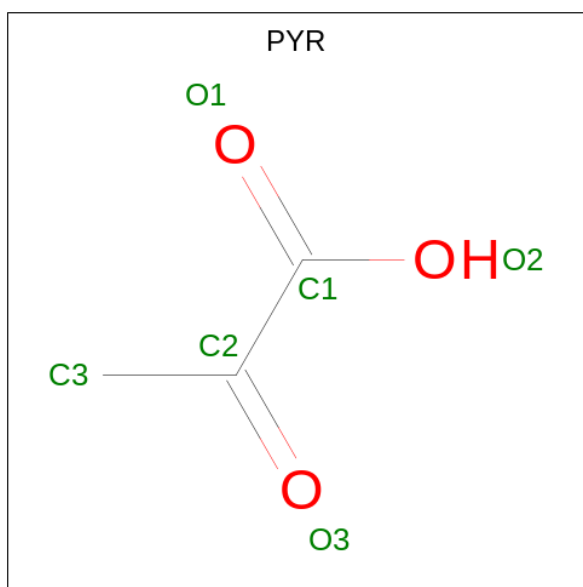
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2841	1795	494	545	7			
1	B	368	Total	C	N	O	S	0	0	0
			2841	1795	494	545	7			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	361	Total	O	0	0
			361	361		
4	B	379	Total	O	0	0
			379	379		

VAL	VAL	ARG	MET	GLY	ASP	LYS	S223	●
ALA	ALA	GLY	PRO	LEU	THR	LYS	P224	●
LEU	ILE	ALA	ILE	ASN	THR	ILE	R225	●
GLY	SER	SER	VAL	GLY	THR	ASP	D226	●
ARG	ILE	GLY	GLN	GLY	VAL	VAL	I227	●
PRO	TRP	TRP	ARG	PRO	ILE	ASN	E228	●
VAL	VAL	VAL	LEU	ARG	LEU	THR	E229	●
PHE	SER	SER	ARG	TRP	GLY	THR	I230	●
GLY	PHE	ASN	GLY	PHE	HIS	ASP	A231	●
LEU	GLY	HIS	THR	GLN	LYS	ASP	A232	●
ALA	ALA	GLY	ALA	TYR	LYS	LEU	E247	+
LEU	LEU	ARG	GLY	MET	ALA	GLU	E251	●
GLY	GLN	GLN	MET	ALA	PRO	GLU	R255	●
TRP	GLY	TYR	LEU	ASP	PHE	ALA	K289	+
GLN	TRP	GLY	LEU	ASP	ILE	SER	R290	+
GLY	GLY	ALA	ASN	GLN	ALA	VAL	S297	+
ALA	PRO	PRO	ILE	ASN	PRO	VAL	D314	+
TYR	GLY	GLY	TYR	ARG	ALA	HIS	V315	+
SER	SER	PHE	GLY	ILE	HIS	GLY	V316	+
LEU	LEU	ASP	SER	LEU	GLY	PHE	P321	+
THR	ASP	THR	LYS	ASP	LEU	ASN	V322	+
PHE	THR	LEU	GLN	GLU	ALA	TYR	L323	+
GLN	PHE	PRO	LYS	ALA	THR	ILE	F324	●
ALA	ASP	ALA	ARG	GLY	LYS	ALA	G325	●
LEU	THR	GLY	ARG	ALA	ALA	SER	L326	●
ARG	VAL	ILE	ASP	ILE	GLY	ASP	A327	●
VAL	ASN	ASN	GLU	THR	THR	GLU	G329	●
MET	VAL	LYS	GLU	ILE	ALA	TRP	L328	●
GLN	ARG	ARG	ILE	ILE	ARG	THR	G330	●
LEU	VAL	VAL	ALA	LEU	ALA	LYS	W331	●
THR	PRO	PRO	ALA	THR	VAL	ARG	Q332	●
GLY	ILE	ILE	HIS	ALA	SER	ALA	G333	●
SER	VAL	VAL	SER	ASP	GLU	ASN	A334	●
GLN	PHE	PHE	GLY	ASP	PHE	ASP	Q355	+
ASN	ASN	ASP	LEU	THR	GLY	ARG	E358	+
VAL	GLY	SER	PRO	VAL	THR	ALA	D367	+
GLU	PHE	GLY	VAL	SER	ILE	TRP	Y370	+
ASP	VAL	VAL	PHE	GLY	MET	LYS	G371	+
LEU	ARG	ARG	VAL	ASN	THR	HIS	Y372	+
GLY	GLY	GLY	LYS	ARG	ILE	LYS	E373	+
LEU	GLY	GLY	ILE	ASP	SER	LEU	Y374	+
ASP	HIS	HIS	GLN	ASP	TYR	TYR	GLU	+
LEU	VAL	VAL	HIS	VAL	SER	ARG	TYR	+
PHE	ALA	ALA	PRO	LYS	GLY	ALA	ASN	+
ASP	ASP	LYS	GLU	ASN	ALA	LEU	ALA	+
ASN	ALA	ALA	ASP	LYS	THR	ALA	GLN	+
PRO	PRO	LEU	ALA	PHE	PHE	GLU	ASP	+
TYR	TYR	ALA	ASP	VAL	GLU	VAL	PRO	+
GLY	SER	SER	MET	THR	ILE	GLU	GLU	+
TYR	GLY	ALA	ALA	PRO	ASP	ALA	GLU	+
GLU	TYR	ILE	ILE	ILE	THR	SER	ILE	+
TYR	ASP	ASP	LYS	GLY	GLU	PRO	PRO	+

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	132.60Å 132.60Å 91.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.93 – 1.41 46.88 – 1.41	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.93-1.41) 99.8 (46.88-1.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.193 , 0.216 0.198 , 0.222	Depositor DCC
R_{free} test set	7774 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6496	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, PYR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	0/2905	0.93	5/3937 (0.1%)
1	B	0.79	2/2905 (0.1%)	0.97	10/3937 (0.3%)
All	All	0.78	2/5810 (0.0%)	0.95	15/7874 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	333	GLY	C-O	10.45	1.40	1.23
1	B	67	LEU	C-O	5.01	1.32	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	TYR	CB-CG-CD2	-9.64	115.22	121.00
1	B	324	PHE	CB-CA-C	8.39	127.18	110.40
1	A	370	TYR	CB-CG-CD1	8.18	125.91	121.00
1	B	370	TYR	CB-CG-CD2	-7.08	116.75	121.00
1	A	374	TYR	CA-C-O	-6.67	106.10	120.10
1	B	370	TYR	CB-CG-CD1	6.62	124.97	121.00
1	B	334	ALA	N-CA-CB	-6.45	101.07	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	GLY	O-C-N	6.29	132.76	122.70
1	B	333	GLY	CA-C-O	-6.15	109.54	120.60
1	A	370	TYR	CG-CD1-CE1	-5.90	116.58	121.30
1	B	374	TYR	CA-C-O	-5.56	108.43	120.10
1	B	334	ALA	N-CA-C	5.17	124.95	111.00
1	B	333	GLY	C-N-CA	5.16	134.60	121.70
1	A	56	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	56	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	ILE	Peptide
1	B	33	VAL	Peptide
1	B	330	GLY	Peptide
1	B	333	GLY	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2841	0	2772	29	0
1	B	2841	0	2772	130	0
2	A	31	0	19	1	0
2	B	31	0	19	0	0
3	A	6	0	3	1	0
3	B	6	0	3	0	0
4	A	361	0	0	9	3
4	B	379	0	0	26	2
All	All	6496	0	5588	158	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (158) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLY:HA3	4:B:932:HOH:O	1.26	1.31
1:B:41:ILE:HD12	1:B:326:LEU:HD22	1.29	1.13
1:B:156:ASP:OD2	1:B:200:ARG:NE	1.83	1.12
1:B:38:PHE:HA	1:B:326:LEU:HD21	1.27	1.11
1:B:33:VAL:HG11	1:B:326:LEU:HA	1.09	1.07
1:B:331:TRP:CE3	4:B:1126:HOH:O	2.06	1.06
1:B:69:GLN:O	4:B:901:HOH:O	1.76	1.03
1:B:38:PHE:CE1	1:B:327:ALA:HB1	1.96	1.01
1:B:325:GLY:HA2	4:B:1126:HOH:O	1.60	1.01
1:B:334:ALA:HB3	4:B:947:HOH:O	1.62	0.99
1:A:251:MET:O	1:A:255:ARG:HG2	1.60	0.99
1:B:33:VAL:CG1	1:B:326:LEU:HA	1.92	0.98
1:B:251:MET:O	1:B:255:ARG:HG2	1.61	0.97
1:B:323:LEU:O	1:B:325:GLY:N	2.01	0.94
1:A:226:ASP:OD2	4:A:901:HOH:O	1.85	0.93
1:B:33:VAL:HG11	1:B:326:LEU:CA	1.98	0.93
1:B:147:MET:O	1:B:219:LYS:CB	2.19	0.90
1:B:27:GLU:O	1:B:329:GLY:N	2.04	0.90
1:B:147:MET:O	1:B:219:LYS:HB3	1.72	0.89
1:B:41:ILE:CD1	1:B:326:LEU:HD22	2.03	0.89
1:B:156:ASP:OD2	1:B:200:ARG:CZ	2.20	0.88
1:B:314:ASP:OD2	4:B:902:HOH:O	1.91	0.88
1:B:41:ILE:HD12	1:B:326:LEU:CD2	2.05	0.86
1:B:38:PHE:CD1	1:B:327:ALA:HA	2.12	0.85
1:B:324:PHE:O	1:B:332:GLN:C	2.18	0.82
1:B:38:PHE:HA	1:B:326:LEU:CD2	2.08	0.82
1:B:29:ALA:H	1:B:330:GLY:N	1.77	0.81
1:B:38:PHE:CE1	1:B:327:ALA:CB	2.64	0.79
1:B:224:PRO:HB3	1:B:255:ARG:HG3	1.63	0.79
1:B:333:GLY:N	4:B:905:HOH:O	2.04	0.78
1:B:38:PHE:CD1	1:B:327:ALA:CB	2.67	0.78
1:B:373:GLU:OE2	4:B:904:HOH:O	2.03	0.76
1:B:226:ASP:O	1:B:230:ILE:HG12	1.86	0.75
1:B:11:PRO:HG3	1:B:33:VAL:HG22	1.68	0.75
1:B:28:GLU:HB3	1:B:330:GLY:O	1.86	0.74
1:B:69:GLN:OE1	4:B:906:HOH:O	2.06	0.74
1:B:26:GLU:O	1:B:327:ALA:HB3	1.87	0.74
1:B:325:GLY:CA	4:B:932:HOH:O	2.00	0.73
1:A:247:GLU:OE2	4:A:902:HOH:O	2.05	0.73
1:B:201:TYR:CZ	1:B:217:ALA:O	2.42	0.72
1:B:333:GLY:C	4:B:905:HOH:O	2.27	0.72
1:B:29:ALA:H	1:B:329:GLY:C	1.92	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:TRP:O	1:B:332:GLN:HG3	1.90	0.72
1:B:30:SER:CB	4:B:903:HOH:O	2.38	0.71
1:B:29:ALA:HB3	1:B:327:ALA:O	1.91	0.70
1:B:333:GLY:O	4:B:905:HOH:O	2.08	0.70
1:B:38:PHE:CD1	1:B:327:ALA:CA	2.75	0.69
1:B:94:ILE:HG21	1:B:323:LEU:HD11	1.75	0.69
1:B:143:PHE:CE2	1:B:145:ILE:HG22	2.27	0.69
1:B:201:TYR:CE1	1:B:217:ALA:O	2.47	0.67
1:B:33:VAL:HB	1:B:326:LEU:O	1.96	0.66
1:B:102:THR:OG1	4:B:907:HOH:O	2.12	0.66
1:B:156:ASP:OD2	1:B:200:ARG:CD	2.43	0.66
1:B:331:TRP:HE3	4:B:1126:HOH:O	1.55	0.65
1:B:17:ILE:HD12	1:B:332:GLN:HB3	1.78	0.64
1:B:143:PHE:HE2	1:B:145:ILE:HG22	1.62	0.64
1:A:73:ALA:N	4:A:908:HOH:O	2.27	0.64
1:B:200:ARG:NH1	4:B:915:HOH:O	2.30	0.63
1:B:77:SER:HB2	1:B:84:LYS:CE	2.27	0.63
1:B:26:GLU:O	1:B:327:ALA:CB	2.47	0.63
1:B:38:PHE:HE1	1:B:327:ALA:HB1	1.55	0.63
1:B:147:MET:O	1:B:219:LYS:HB2	1.97	0.62
1:B:147:MET:HG2	1:B:171:LEU:HD11	1.81	0.61
1:B:29:ALA:HB3	1:B:327:ALA:N	2.15	0.61
1:B:147:MET:HE3	1:B:154:ASN:HD21	1.66	0.61
1:B:30:SER:OG	4:B:903:HOH:O	1.95	0.60
1:B:324:PHE:O	1:B:332:GLN:O	2.19	0.60
1:B:147:MET:CE	1:B:154:ASN:HD21	2.14	0.59
1:B:147:MET:SD	1:B:226:ASP:OD1	2.60	0.59
1:A:61:LYS:NZ	1:A:367:ASP:OD1	2.25	0.59
1:A:224:PRO:HB3	1:A:255:ARG:HG3	1.84	0.58
1:B:29:ALA:CB	1:B:326:LEU:C	2.72	0.58
1:B:29:ALA:HB2	1:B:331:TRP:HA	1.85	0.57
1:B:333:GLY:CA	4:B:905:HOH:O	2.52	0.57
1:B:38:PHE:CE2	1:B:328:LEU:HD13	2.39	0.57
1:B:38:PHE:CA	1:B:326:LEU:HD21	2.19	0.57
1:B:77:SER:HB2	1:B:84:LYS:HE2	1.85	0.57
1:B:202:LEU:O	1:B:204:GLY:N	2.38	0.56
1:B:147:MET:HE3	1:B:154:ASN:ND2	2.20	0.56
1:B:289:LYS:NZ	4:B:918:HOH:O	2.39	0.55
1:B:251:MET:HG2	1:B:255:ARG:HE	1.71	0.54
1:B:30:SER:H	1:B:328:LEU:C	2.10	0.54
1:B:147:MET:SD	1:B:226:ASP:HB3	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:GLU:O	1:B:29:ALA:CB	2.55	0.54
1:A:224:PRO:HA	1:A:227:ILE:HD12	1.90	0.53
1:B:30:SER:H	1:B:329:GLY:N	2.06	0.53
1:B:147:MET:CE	1:B:154:ASN:ND2	2.72	0.52
1:B:331:TRP:O	1:B:332:GLN:CG	2.56	0.52
1:B:25:LEU:HD22	1:B:332:GLN:HB3	1.92	0.52
1:B:222:ILE:HD11	4:B:957:HOH:O	2.09	0.52
1:A:225:ARG:NH1	4:A:917:HOH:O	2.42	0.51
1:B:27:GLU:O	1:B:328:LEU:HB3	2.10	0.51
1:B:149:LYS:NZ	1:B:216:GLY:O	2.43	0.51
1:B:77:SER:HB2	1:B:84:LYS:HE3	1.92	0.51
1:B:94:ILE:HG21	1:B:323:LEU:CD1	2.41	0.51
1:B:30:SER:HB2	4:B:903:HOH:O	2.08	0.51
1:B:29:ALA:HA	1:B:331:TRP:N	2.26	0.51
1:B:30:SER:HB3	1:B:328:LEU:CA	2.41	0.51
1:B:29:ALA:HB3	1:B:326:LEU:C	2.30	0.51
1:A:153:GLN:OE1	1:A:201:TYR:HB3	2.11	0.50
1:B:29:ALA:O	1:B:33:VAL:CG2	2.60	0.50
1:B:247:GLU:OE2	4:B:909:HOH:O	2.20	0.50
1:B:29:ALA:HB1	1:B:326:LEU:C	2.32	0.50
1:B:367:ASP:OD2	4:B:908:HOH:O	2.19	0.50
1:B:225:ARG:O	1:B:229:GLU:N	2.39	0.50
1:B:324:PHE:O	1:B:333:GLY:N	2.44	0.50
1:B:323:LEU:O	1:B:324:PHE:C	2.51	0.50
1:B:29:ALA:N	1:B:330:GLY:N	2.55	0.49
1:B:11:PRO:HG2	1:B:325:GLY:O	2.12	0.49
1:A:181:ARG:HD3	4:A:922:HOH:O	2.13	0.48
1:B:15:LYS:HG2	1:B:331:TRP:CZ2	2.49	0.48
1:B:225:ARG:HB2	4:B:912:HOH:O	2.13	0.48
1:A:66:ARG:C	1:A:67:LEU:HD23	2.34	0.48
1:A:285:GLU:OE1	4:A:903:HOH:O	2.20	0.47
1:B:29:ALA:O	1:B:33:VAL:HG23	2.15	0.47
1:B:33:VAL:CG1	1:B:326:LEU:O	2.62	0.47
1:B:38:PHE:CD1	1:B:327:ALA:HB2	2.50	0.47
1:B:147:MET:HE2	1:B:219:LYS:CD	2.45	0.47
1:A:251:MET:O	1:A:255:ARG:CG	2.49	0.46
1:B:33:VAL:CB	1:B:326:LEU:O	2.63	0.46
1:B:147:MET:HE2	1:B:219:LYS:HD3	1.96	0.46
1:B:199:GLN:HA	1:B:199:GLN:OE1	2.15	0.46
1:A:164:ASP:HB2	4:A:905:HOH:O	2.16	0.46
1:A:89:PHE:HA	1:A:316:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ALA:HB1	1:A:136:LEU:CD2	2.47	0.45
1:B:100:ALA:O	1:B:325:GLY:O	2.35	0.45
1:A:224:PRO:HG3	1:A:251:MET:SD	2.56	0.45
1:B:129:PHE:CE1	1:B:164:ASP:HB3	2.51	0.45
1:B:148:ALA:O	1:B:219:LYS:HD2	2.17	0.44
1:B:27:GLU:HA	1:B:328:LEU:CB	2.48	0.44
1:B:89:PHE:HA	1:B:316:VAL:O	2.18	0.44
1:B:17:ILE:HG21	1:B:332:GLN:HG2	2.00	0.43
1:B:223:SER:O	1:B:226:ASP:HB2	2.18	0.43
1:A:199:GLN:HB3	4:A:909:HOH:O	2.17	0.43
1:B:25:LEU:CD2	1:B:332:GLN:HB3	2.48	0.43
1:B:147:MET:HE2	1:B:147:MET:HB3	1.80	0.43
1:B:176:THR:HB	1:B:220:GLN:HA	2.01	0.43
1:A:148:ALA:HB2	1:A:201:TYR:CD2	2.54	0.43
1:A:171:LEU:HD22	1:A:230:ILE:HD12	2.01	0.42
1:A:358:GLU:O	1:B:290:ARG:HD3	2.19	0.42
1:B:30:SER:HB3	1:B:328:LEU:C	2.39	0.42
1:A:290:ARG:HD3	1:B:358:GLU:O	2.18	0.42
1:B:38:PHE:HA	1:B:326:LEU:CG	2.50	0.42
1:B:331:TRP:CD2	4:B:1084:HOH:O	2.73	0.42
1:B:224:PRO:HB3	1:B:255:ARG:CG	2.42	0.42
1:B:38:PHE:CG	1:B:327:ALA:HA	2.55	0.42
1:A:273:ALA:HB1	1:A:274:PRO:HD2	2.02	0.41
1:A:241:LYS:HA	1:A:261:TRP:HB3	2.03	0.41
1:B:22:THR:HB	1:B:321:PRO:HB3	2.02	0.41
1:A:67:LEU:HD23	1:A:67:LEU:N	2.36	0.41
2:A:801:FMN:N5	3:A:802:PYR:C2	2.84	0.41
1:A:231:ALA:HB1	4:A:997:HOH:O	2.21	0.41
1:A:309:LEU:HD23	1:A:357:VAL:HG13	2.02	0.41
1:B:372:TYR:N	4:B:931:HOH:O	2.53	0.41
1:B:27:GLU:HA	1:B:328:LEU:HB2	2.02	0.41
1:B:71:VAL:HG22	1:B:355:GLN:HB2	2.03	0.41
1:A:225:ARG:O	1:A:228:GLU:HB2	2.22	0.40
1:A:309:LEU:CD2	1:A:357:VAL:HG13	2.51	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1216:HOH:O	4:A:1216:HOH:O[3_655]	1.88	0.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1150:HOH:O	4:A:1150:HOH:O[3_655]	1.92	0.28
4:B:1235:HOH:O	4:B:1235:HOH:O[3_655]	1.95	0.25
4:B:1043:HOH:O	4:B:1043:HOH:O[3_655]	1.99	0.21
4:A:1019:HOH:O	4:A:1019:HOH:O[3_655]	2.03	0.17

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	366/736 (50%)	355 (97%)	9 (2%)	2 (0%)	29	8
1	B	366/736 (50%)	343 (94%)	15 (4%)	8 (2%)	6	0
All	All	732/1472 (50%)	698 (95%)	24 (3%)	10 (1%)	11	1

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ARG
1	A	297	SER
1	B	200	ARG
1	B	297	SER
1	B	324	PHE
1	B	328	LEU
1	B	334	ALA
1	B	29	ALA
1	B	203	ARG
1	B	211	LEU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	292/584 (50%)	288 (99%)	4 (1%)	67	38
1	B	292/584 (50%)	283 (97%)	9 (3%)	40	9
All	All	584/1168 (50%)	571 (98%)	13 (2%)	52	18

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	ARG
1	A	199	GLN
1	A	203	ARG
1	A	224	PRO
1	B	141	ARG
1	B	147	MET
1	B	153	GLN
1	B	195	MET
1	B	199	GLN
1	B	201	TYR
1	B	224	PRO
1	B	225	ARG
1	B	328	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	199	GLN
1	B	35	HIS
1	B	153	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PYR	A	802	-	2,5,5	0.87	0	2,6,6	1.20	0
3	PYR	B	802	-	2,5,5	0.34	0	2,6,6	1.49	0
2	FMN	A	801	-	31,33,33	1.37	2 (6%)	40,50,50	2.37	7 (17%)
2	FMN	B	801	-	31,33,33	1.37	3 (9%)	40,50,50	2.10	6 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PYR	A	802	-	-	0/0/4/4	-
3	PYR	B	802	-	-	0/0/4/4	-
2	FMN	A	801	-	-	2/18/18/18	0/3/3/3
2	FMN	B	801	-	-	1/18/18/18	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FMN	C4A-C10	5.60	1.44	1.38
2	B	801	FMN	C4A-C10	4.82	1.43	1.38
2	B	801	FMN	C4-N3	3.13	1.38	1.33
2	A	801	FMN	C4-N3	2.76	1.37	1.33
2	B	801	FMN	C2-N1	-2.55	1.33	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FMN	C2-N3-C4	9.19	122.90	115.14
2	B	801	FMN	C2-N3-C4	7.67	121.62	115.14
2	A	801	FMN	C10-C4A-C4	-6.52	115.64	119.95
2	B	801	FMN	C10-C4A-C4	-5.91	116.04	119.95
2	A	801	FMN	C10-C4A-N5	5.85	125.31	121.26
2	B	801	FMN	C10-C4A-N5	4.86	124.62	121.26
2	A	801	FMN	C4A-C4-N3	-4.43	117.37	123.43
2	B	801	FMN	C4A-C4-N3	-4.17	117.72	123.43
2	A	801	FMN	C4A-C10-N10	-3.98	116.21	120.30
2	B	801	FMN	C4A-C10-N10	-3.91	116.28	120.30
2	A	801	FMN	C5A-C9A-N10	2.24	119.34	117.72
2	A	801	FMN	O5'-C5'-C4'	2.24	115.34	109.36
2	B	801	FMN	C1'-N10-C9A	2.08	119.93	118.29

There are no chirality outliers.

All (3) torsion outliers are listed below:

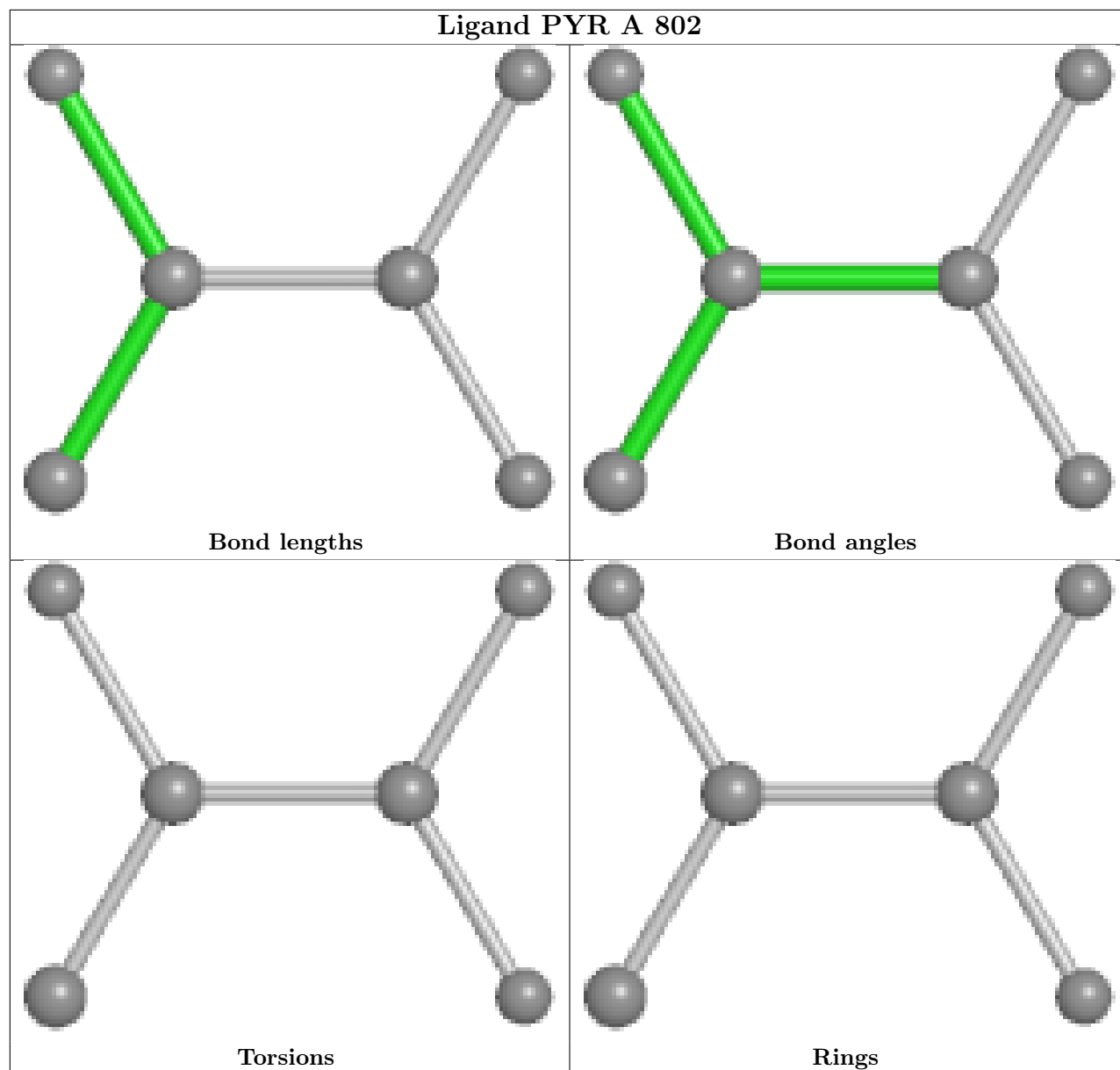
Mol	Chain	Res	Type	Atoms
2	A	801	FMN	C5'-O5'-P-O1P
2	A	801	FMN	C4'-C5'-O5'-P
2	B	801	FMN	C4'-C5'-O5'-P

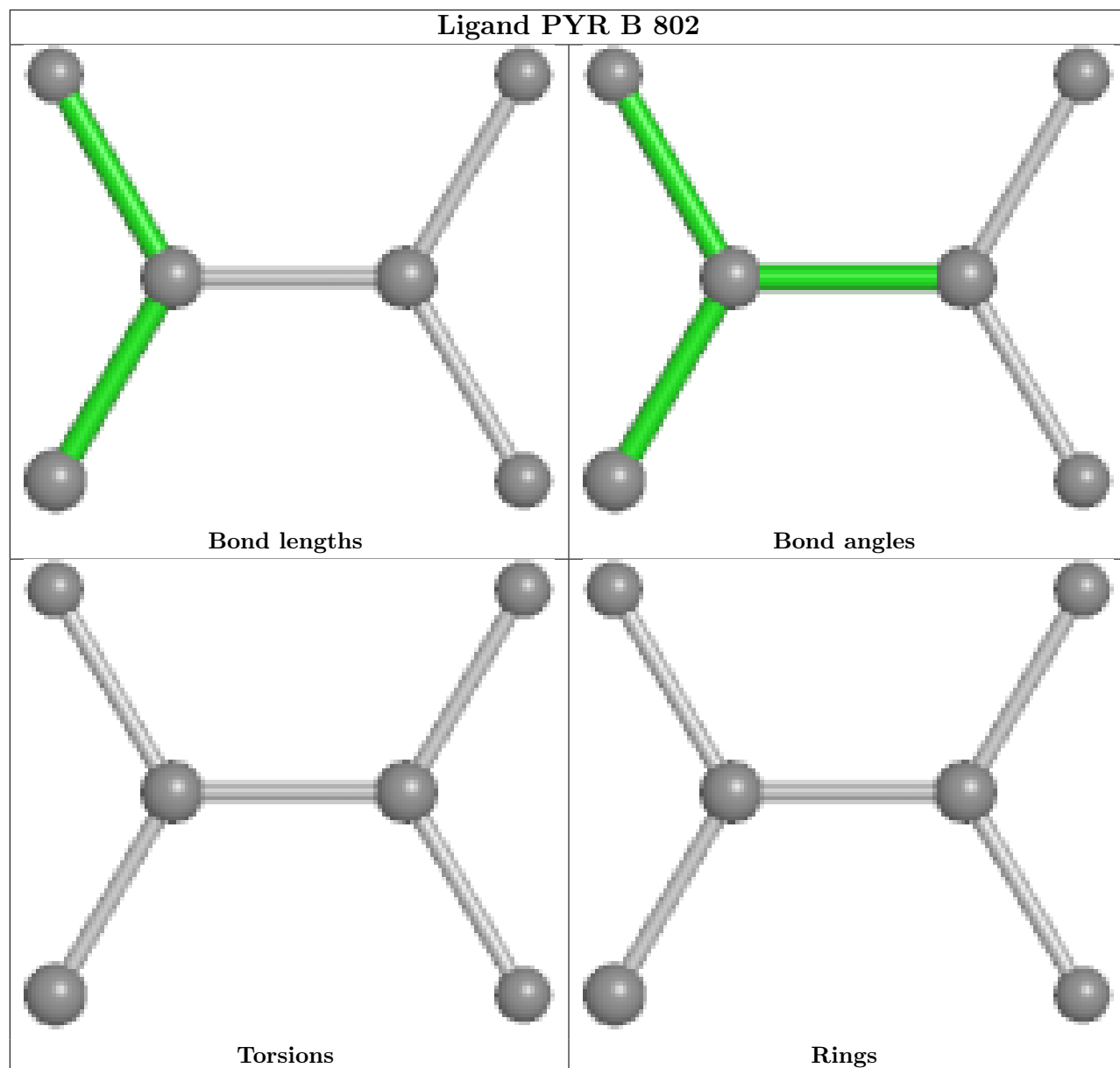
There are no ring outliers.

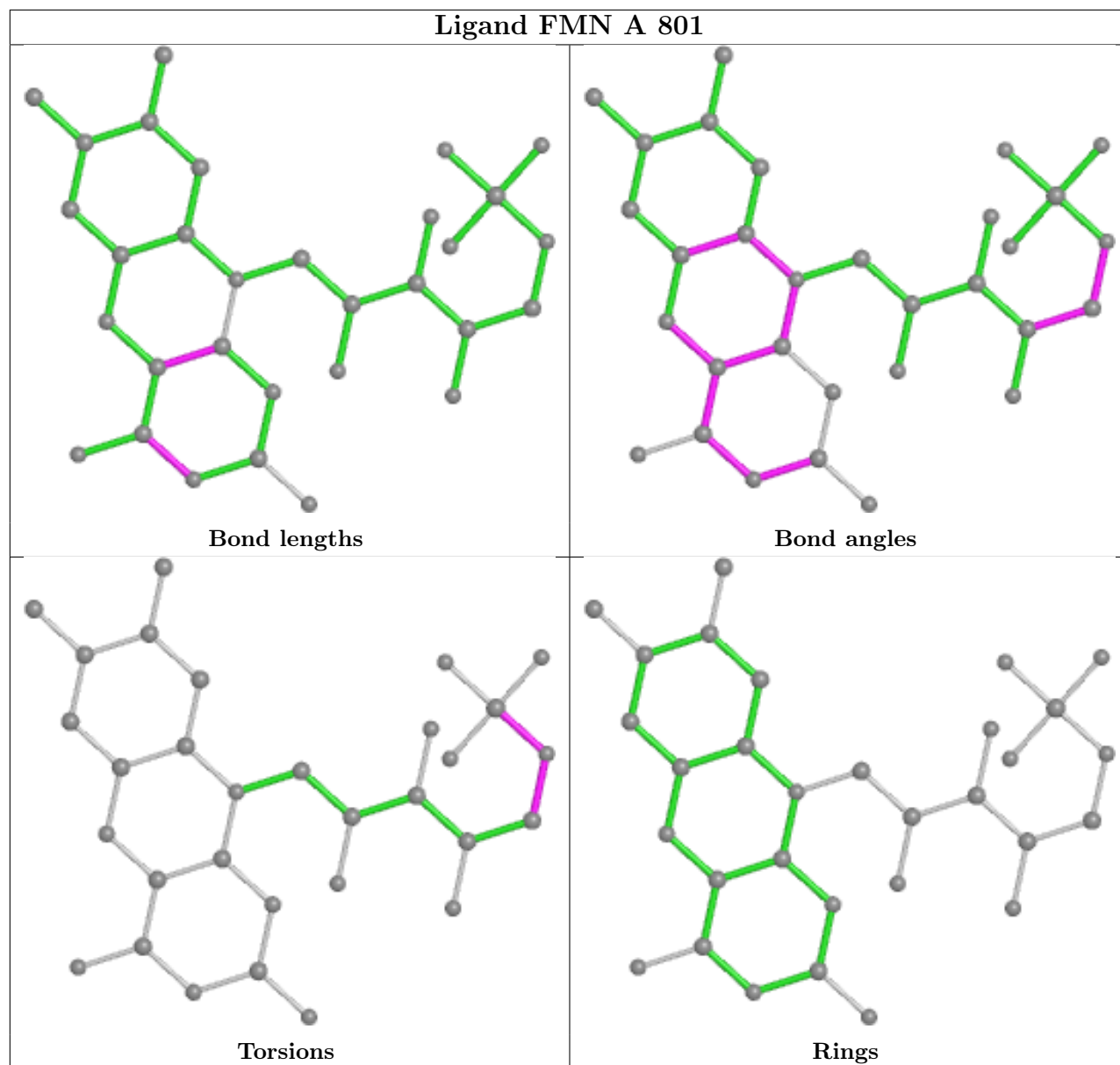
2 monomers are involved in 1 short contact:

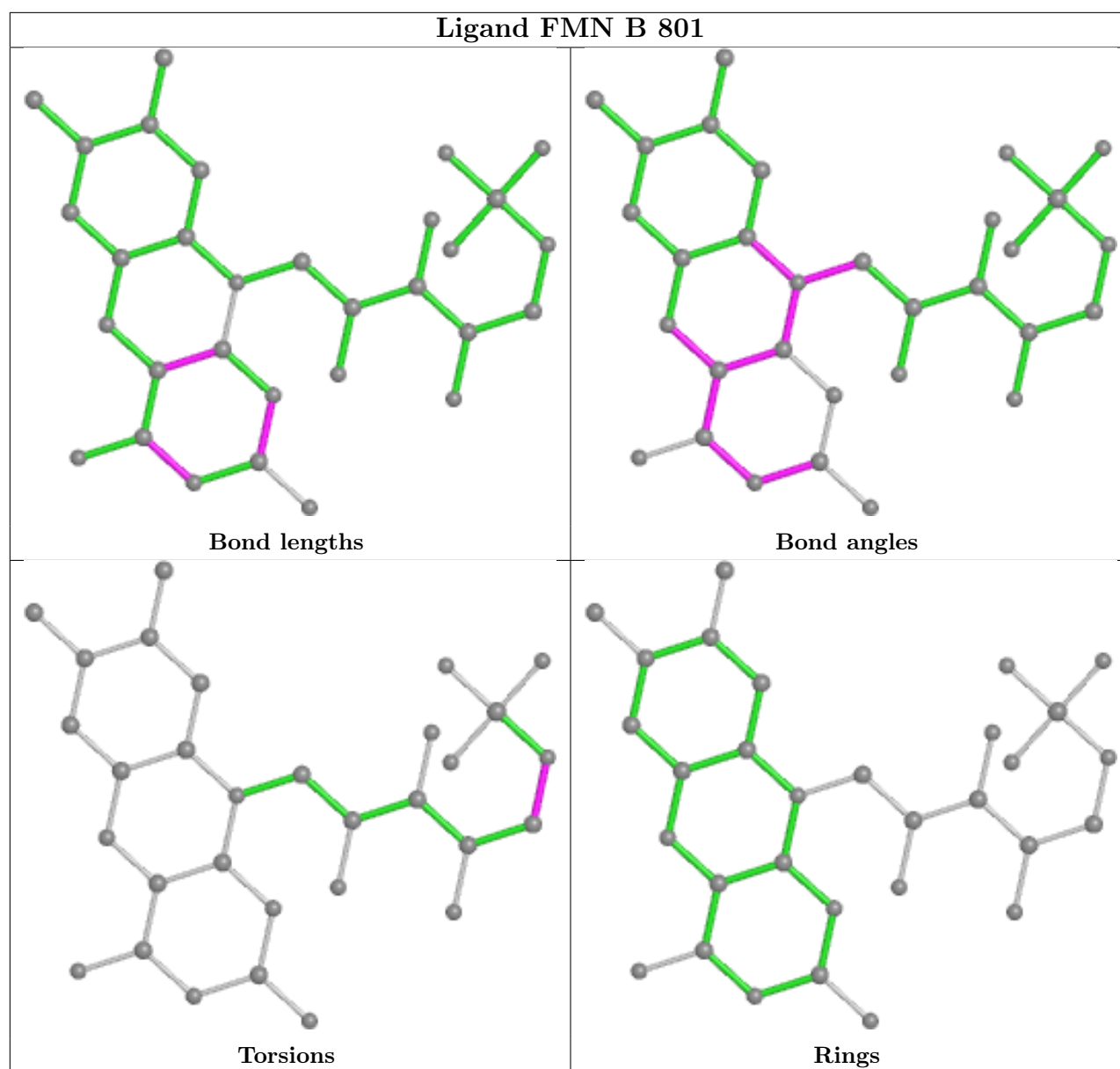
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	PYR	1	0
2	A	801	FMN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	368/736 (50%)	1.25	70 (19%) 1 0	12, 20, 44, 119	0
1	B	368/736 (50%)	2.62	82 (22%) 0 0	12, 20, 93, 206	0
All	All	736/1472 (50%)	1.93	152 (20%) 1 0	12, 20, 62, 206	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	211	LEU	71.5
1	B	326	LEU	43.5
1	B	330	GLY	40.5
1	B	32	VAL	40.1
1	B	206	ALA	37.1
1	B	331	TRP	34.6
1	B	201	TYR	28.8
1	B	210	SER	26.6
1	B	202	LEU	22.4
1	B	209	MET	21.1
1	B	216	GLY	20.8
1	B	332	GLN	20.4
1	A	203	ARG	20.0
1	B	327	ALA	15.4
1	B	328	LEU	15.1
1	B	30	SER	15.1
1	B	207	GLU	14.8
1	B	203	ARG	14.5
1	B	212	ASN	13.8
1	B	214	ILE	13.8
1	A	205	THR	13.7
1	B	215	TYR	13.6
1	B	213	ASN	12.6
1	B	329	GLY	11.7

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Mol	Chain	Res	Type	RSRZ
1	B	208	GLY	11.6
1	A	204	GLY	11.4
1	B	29	ALA	11.2
1	B	205	THR	11.1
1	B	204	GLY	10.9
1	B	325	GLY	10.8
1	B	33	VAL	10.5
1	B	200	ARG	10.1
1	B	185	VAL	9.7
1	B	333	GLY	9.5
1	A	215	TYR	9.2
1	A	202	LEU	8.8
1	B	31	LYS	8.5
1	A	214	ILE	7.9
1	B	222	ILE	7.3
1	B	73	ALA	6.9
1	A	208	GLY	6.8
1	A	199	GLN	6.8
1	A	189	PHE	6.7
1	B	177	VAL	6.6
1	A	201	TYR	6.5
1	A	67	LEU	6.5
1	A	7	GLU	6.5
1	B	67	LEU	6.5
1	A	198	VAL	6.5
1	A	212	ASN	6.2
1	B	199	GLN	6.1
1	B	190	VAL	6.1
1	A	129	PHE	6.1
1	B	191	TYR	6.0
1	A	211	LEU	5.8
1	A	157	ILE	5.8
1	A	227	ILE	5.7
1	A	193	PHE	5.6
1	A	200	ARG	5.6
1	A	197	ILE	5.6
1	A	230	ILE	5.4
1	A	216	GLY	5.3
1	A	222	ILE	5.3
1	B	220	GLN	5.3
1	B	68	ALA	5.2
1	B	232	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	176	THR	5.0
1	A	191	TYR	5.0
1	B	189	PHE	4.7
1	A	232	ALA	4.6
1	B	178	SER	4.6
1	B	188	LYS	4.5
1	A	206	ALA	4.4
1	A	177	VAL	4.4
1	A	185	VAL	4.2
1	A	190	VAL	4.2
1	A	209	MET	4.2
1	B	334	ALA	4.2
1	A	161	ALA	4.1
1	A	176	THR	4.1
1	B	193	PHE	4.1
1	B	198	VAL	4.0
1	B	225	ARG	4.0
1	A	143	PHE	3.9
1	A	207	GLU	3.8
1	A	163	SER	3.8
1	B	218	SER	3.8
1	A	225	ARG	3.7
1	B	18	ASP	3.7
1	A	158	LEU	3.7
1	A	213	ASN	3.7
1	B	223	SER	3.6
1	A	148	ALA	3.6
1	B	186	LYS	3.5
1	B	71	VAL	3.4
1	A	68	ALA	3.4
1	A	192	PRO	3.3
1	B	7	GLU	3.3
1	A	188	LYS	3.3
1	A	153	GLN	3.3
1	B	217	ALA	3.2
1	A	231	ALA	3.2
1	A	146	TYR	3.2
1	B	143	PHE	3.2
1	B	179	GLY	3.1
1	B	38	PHE	3.1
1	B	157	ILE	3.0
1	B	221	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	156	ASP	3.0
1	B	194	GLY	2.9
1	A	220	GLN	2.9
1	B	255	ARG	2.9
1	A	9	ASN	2.9
1	A	134	GLU	2.9
1	B	147	MET	2.9
1	B	187	ASN	2.8
1	A	210	SER	2.8
1	B	251	MET	2.8
1	A	145	ILE	2.7
1	B	72	GLU	2.7
1	A	217	ALA	2.7
1	B	224	PRO	2.7
1	A	234	SER	2.7
1	A	186	LYS	2.6
1	A	218	SER	2.6
1	B	124	TYR	2.5
1	A	159	ASP	2.5
1	A	255	ARG	2.5
1	A	137	ASN	2.5
1	B	227	ILE	2.4
1	A	150	ASP	2.4
1	B	184	ASP	2.4
1	A	228	GLU	2.4
1	A	82	GLY	2.4
1	A	147	MET	2.4
1	B	69	GLN	2.3
1	B	183	ARG	2.2
1	A	194	GLY	2.2
1	A	71	VAL	2.2
1	A	224	PRO	2.2
1	B	129	PHE	2.1
1	A	251	MET	2.1
1	A	178	SER	2.1
1	A	184	ASP	2.1
1	B	62	LEU	2.1
1	B	134	GLU	2.1
1	B	230	ILE	2.0
1	A	195	MET	2.0
1	B	182	ASP	2.0
1	B	228	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	195	MET	2.0
1	B	226	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

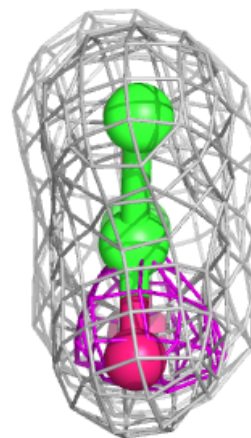
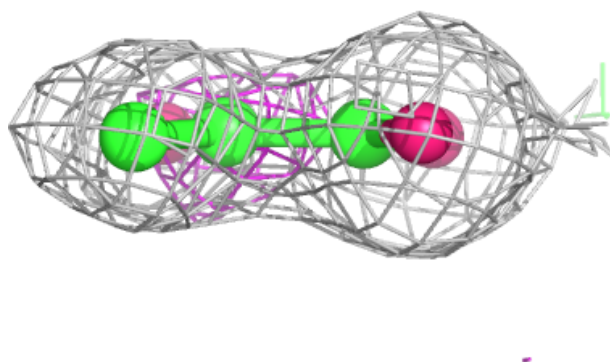
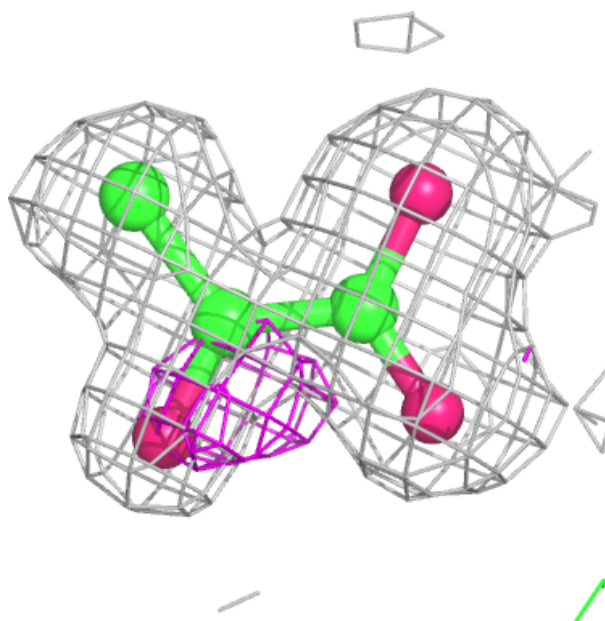
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PYR	A	802	6/6	0.81	0.14	24,26,28,30	0
3	PYR	B	802	6/6	0.83	0.17	26,28,29,31	0
2	FMN	A	801	31/31	0.96	0.08	13,15,18,19	0
2	FMN	B	801	31/31	0.96	0.09	13,15,18,18	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

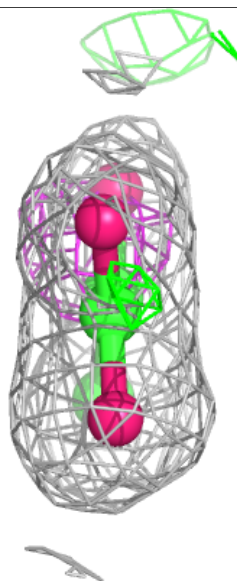
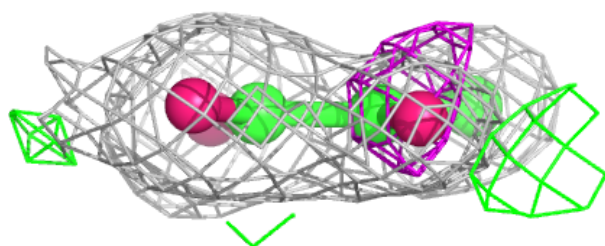
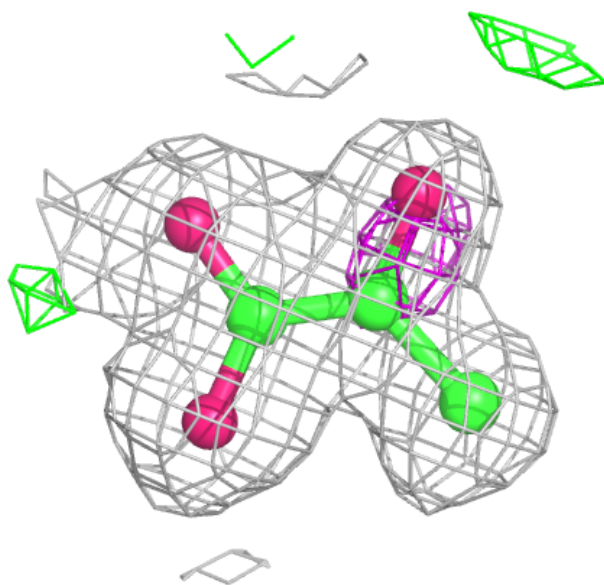
Electron density around PYR A 802:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



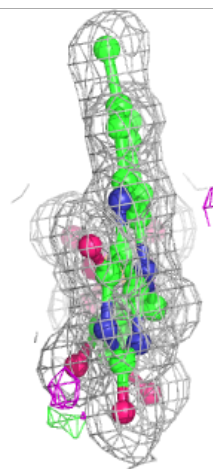
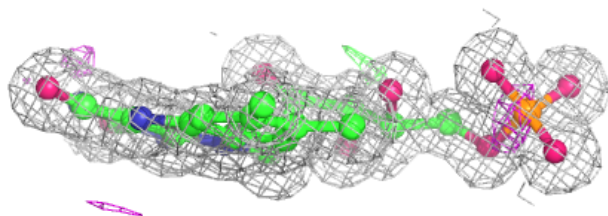
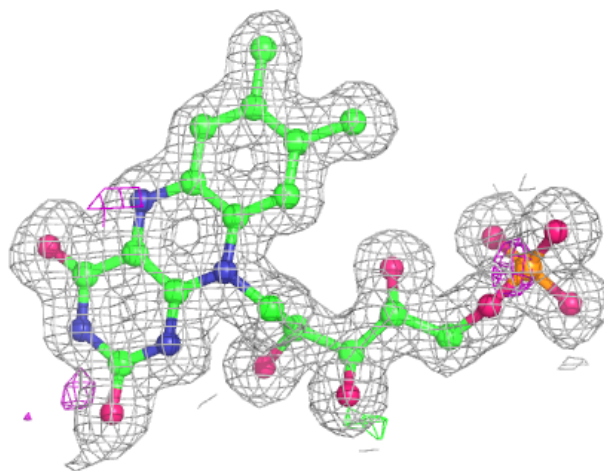
Electron density around PYR B 802:

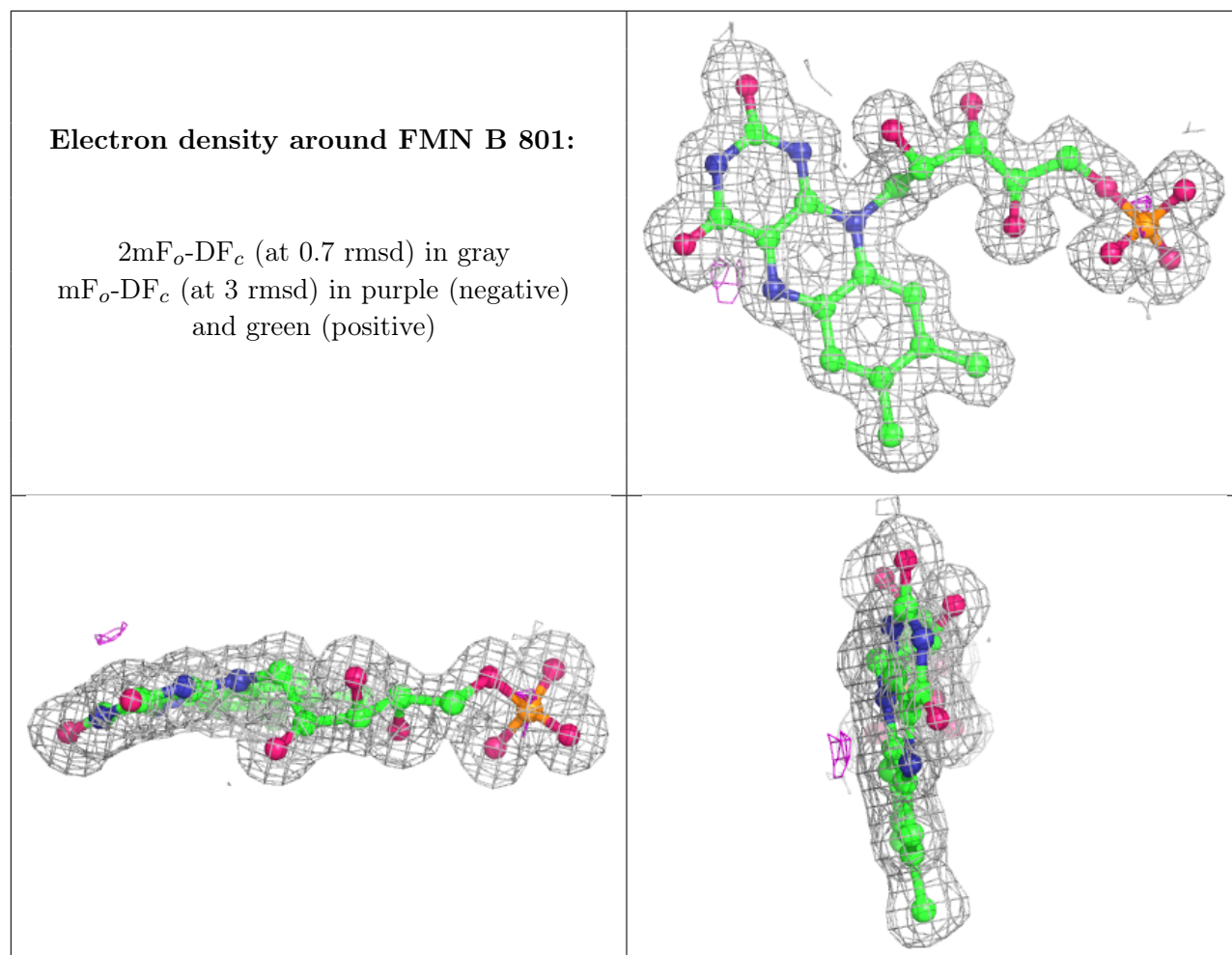
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN A 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.